


Direct Simulation Monte Carlo Calculations in support of the Columbia Shuttle Orbiter Accident Investigation



Michael A. Gallis
Sandia National Laboratories

Gerald J. LeBeau & Katie A. Boyles
NASA Johnson Space Center

Fifth Biennial Tri-Laboratory Engineering Conference
October 21-23, 2003
Santa Fe, NM



Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.

Mathematical models for gas dynamics



$$Kn = \lambda / L$$



λ : local mean free path
L: characteristic length

Euler Equations	Navier-Stokes Equations	Conservation Equations do not form a closed set
Boltzmann Equation		Collisionless Boltzmann Equation

0 0.01 1 100

Local Knudsen number








The Boltzmann Equation



$$\frac{\partial}{\partial t}(nf) + \vec{v} \cdot \frac{\partial}{\partial \vec{r}}(nf) + \vec{F} \cdot \frac{\partial}{\partial \vec{v}}(nf) = \left[\frac{\partial}{\partial t}(nf) \right]_{\text{collision}}$$

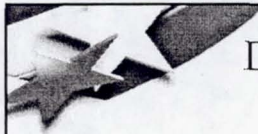
f : distribution function
n : number density
F : external force


Microscopic description of gases

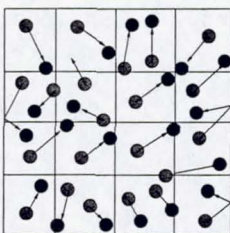
- The rarefied regime is described by the Boltzmann equation
- Particulate nature of gas
- Gas is described by the position, velocity, energy of an ensemble of molecules in a statistical manner
- The microscopic description describes physical processes regardless of the mathematical complexity of the problem



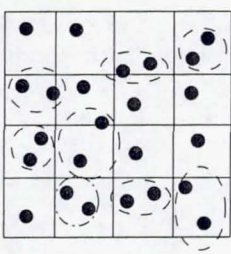
Direct Simulation Monte Carlo (DSMC)







Move phase (deterministic)


$$\frac{\partial}{\partial t}(nf) + \vec{v} \cdot \frac{\partial}{\partial \vec{r}}(nf) + \vec{F} \cdot \frac{\partial}{\partial \vec{v}}(nf) = 0$$




Collide phase (stochastic)

$$\frac{\partial}{\partial t}(nf) = \left[\frac{\partial}{\partial t}(nf) \right]_{\text{collision}}$$








DSMC methodology



- Physical statistical simulation of real dilute gas flow
- Millions of molecules representing real gas molecules modify their velocities and positions as they interact with each other and the boundaries
- Discretization of time and physical space
- Decoupling of the move and the collide phase



Features of DSMC



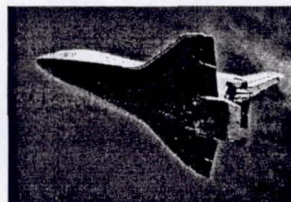
- The calculation is always unsteady. Steady state achieved as a long time state of the unsteady flow
- There are no *numerical instabilities*
- Fluctuations have the same physical characteristics as the real fluctuations
- Physics and chemistry models are mere additions to the molecular model (*surface interactions, energy exchange, chemical reactions*)



Application overview



- Ultimate goal: *to provide "piecewise integration" of key scenario events to determine the plausibility or implausibility of the candidate failure scenarios*
- Target of current analysis: Determine aerodynamic and heating behavior of the Shuttle Orbiter during aerobraking maneuvers
 - Provide an independent assessment of the internal plume engineering model developed by Steve Fitzgerald (NASA JSC)
- Methodology: Direct Simulation Monte Carlo method
 - DAC implementation by LeBeau (NASA JSC)
- Results: Flowfield simulations at representative re-entry trajectory points

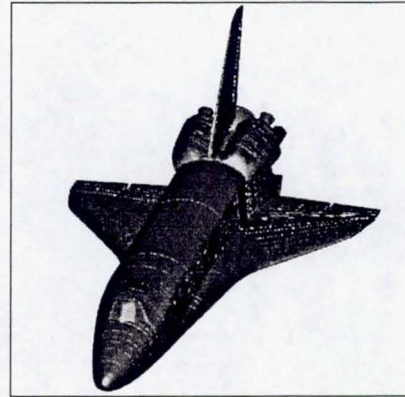




Modeling procedure



- Geometry Modeling
 - Surface grid: Triangulated unstructured constructed from Orbiter CAD model
 - Gas phase grid: Cartesian (adapted where large gradients are present)
- 3-D DSMC Analysis
 - Code used: DAC (version 97)
 - Thermal and chemical non-equilibrium included
 - Chemistry modeling : Finite rate chemistry model of Bird



CAD model for the Orbiter

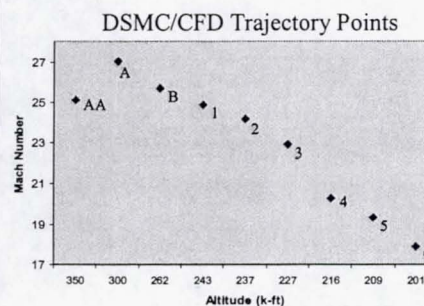


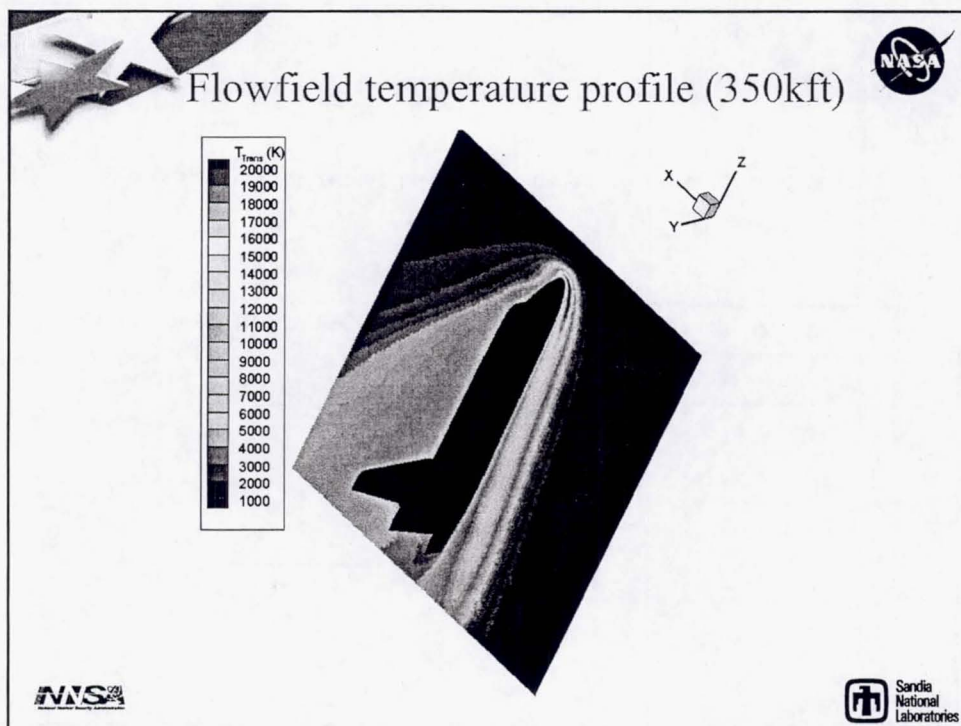
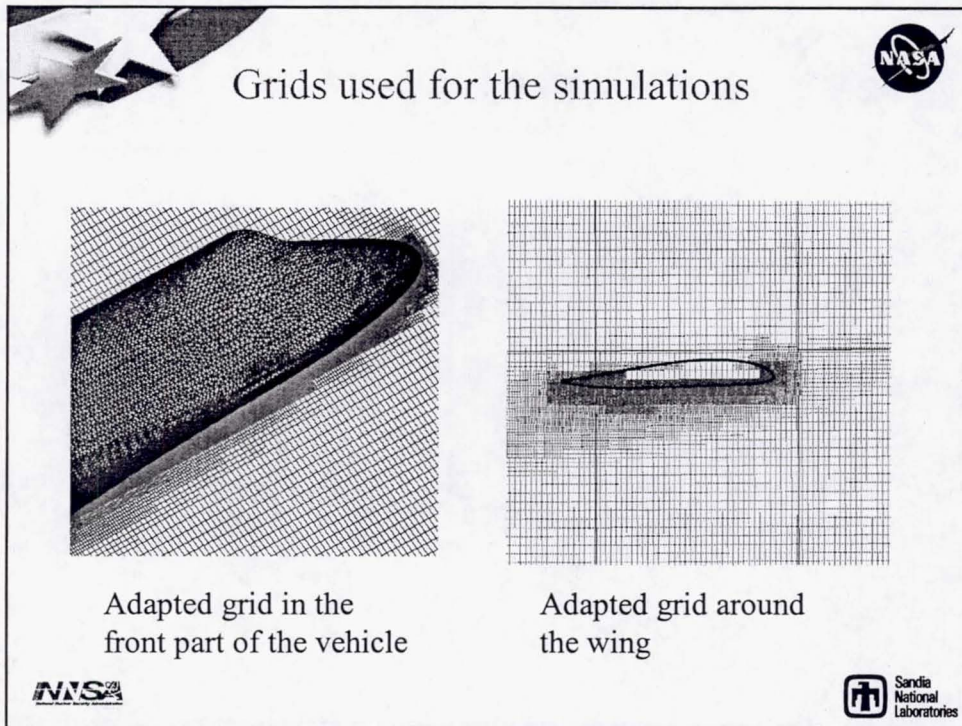
DSMC analysis of flight trajectory

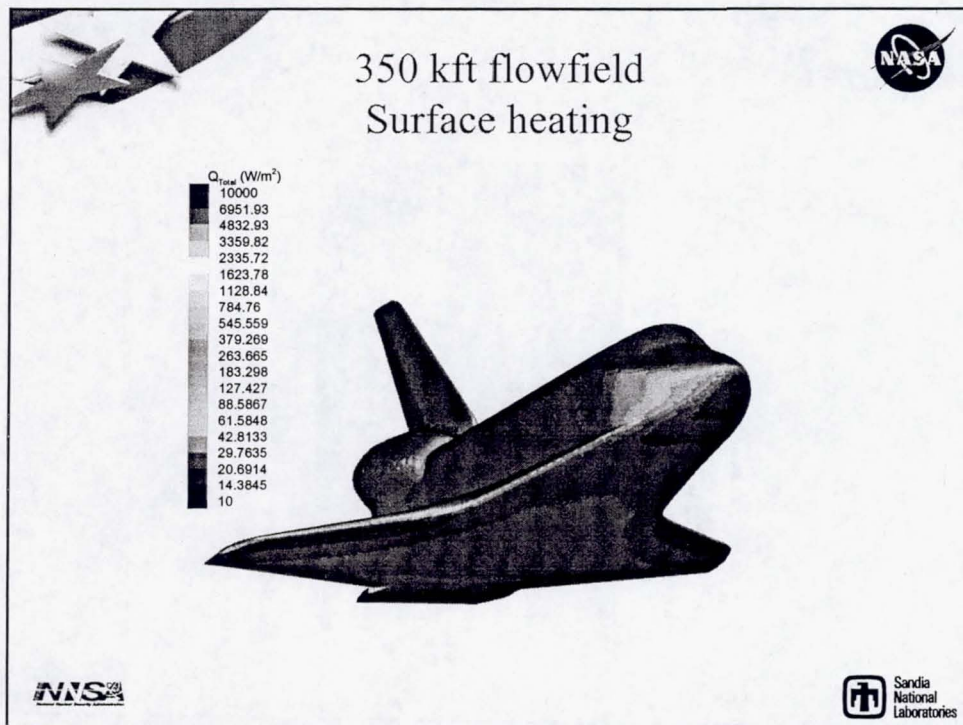
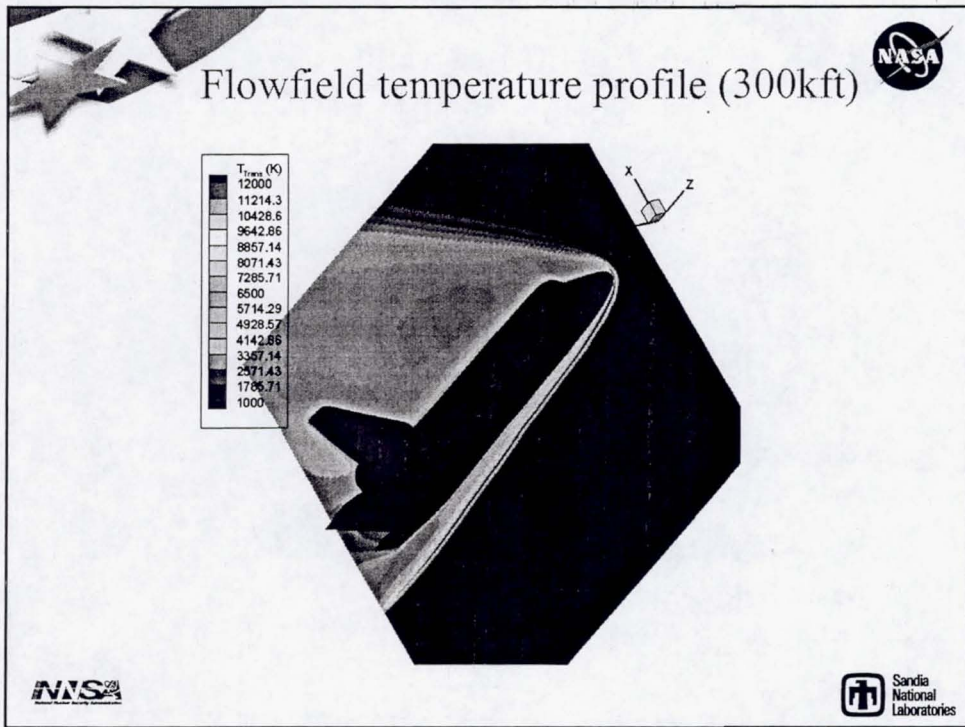


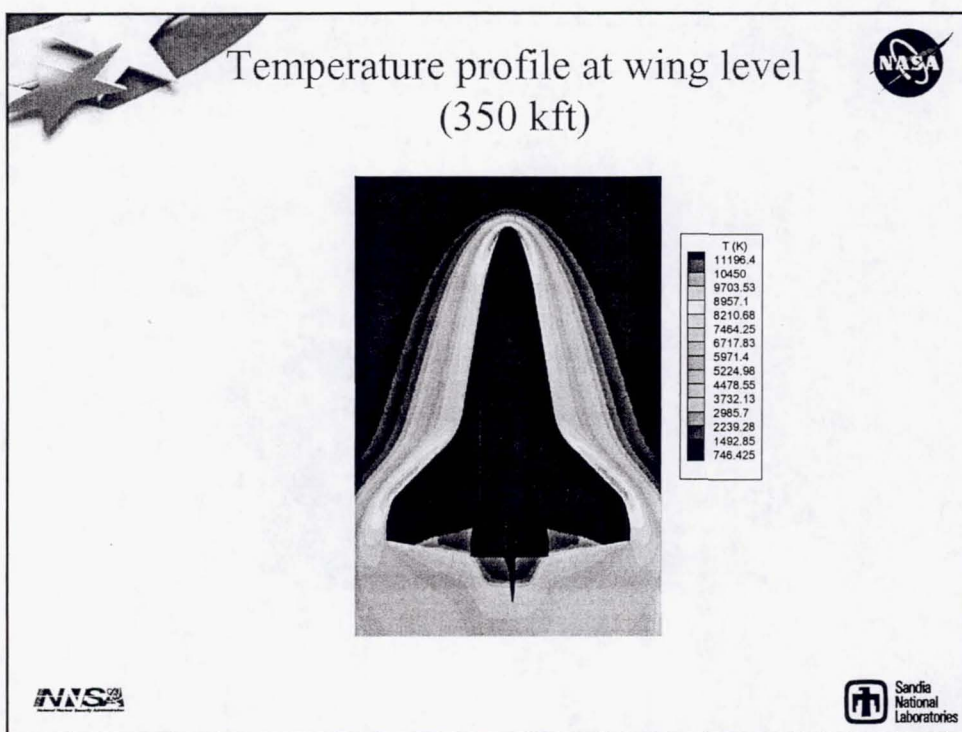
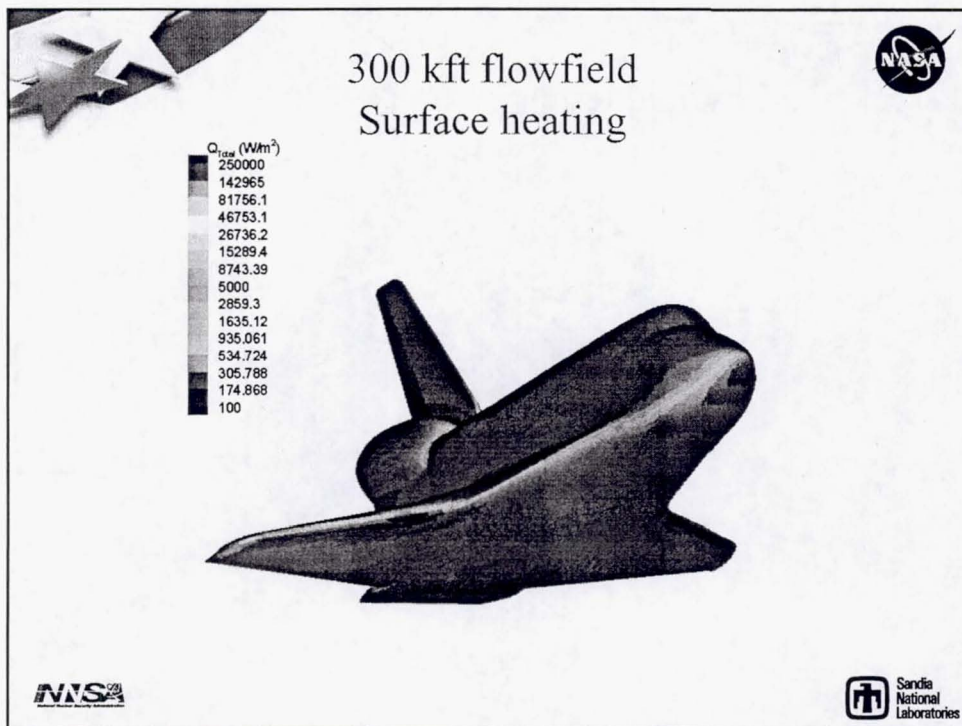
- DSMC simulations were performed at two points of the entry trajectory

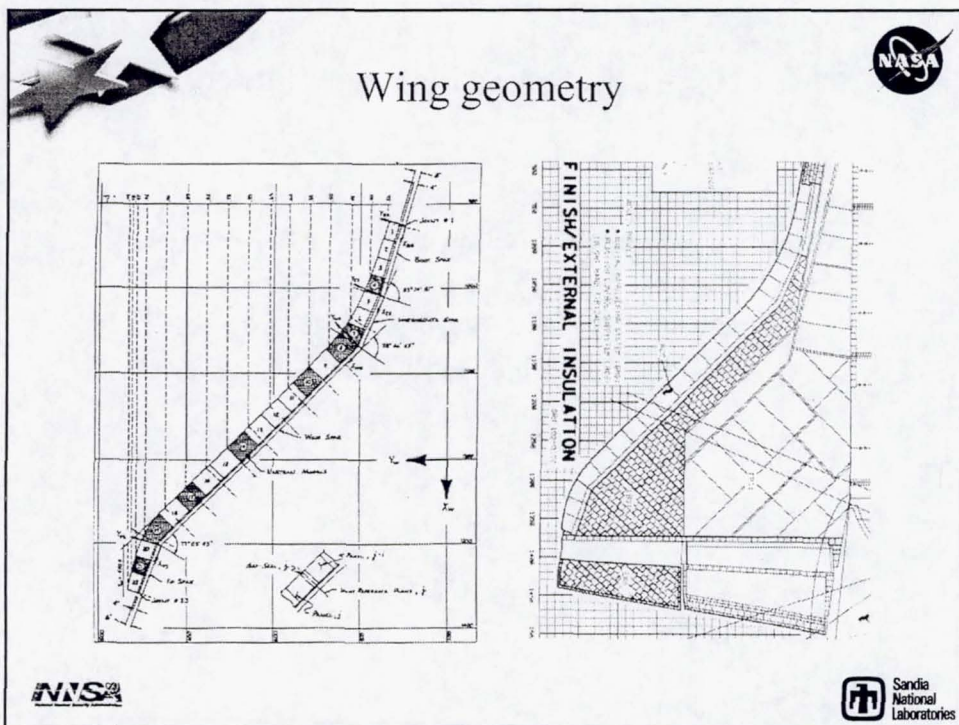
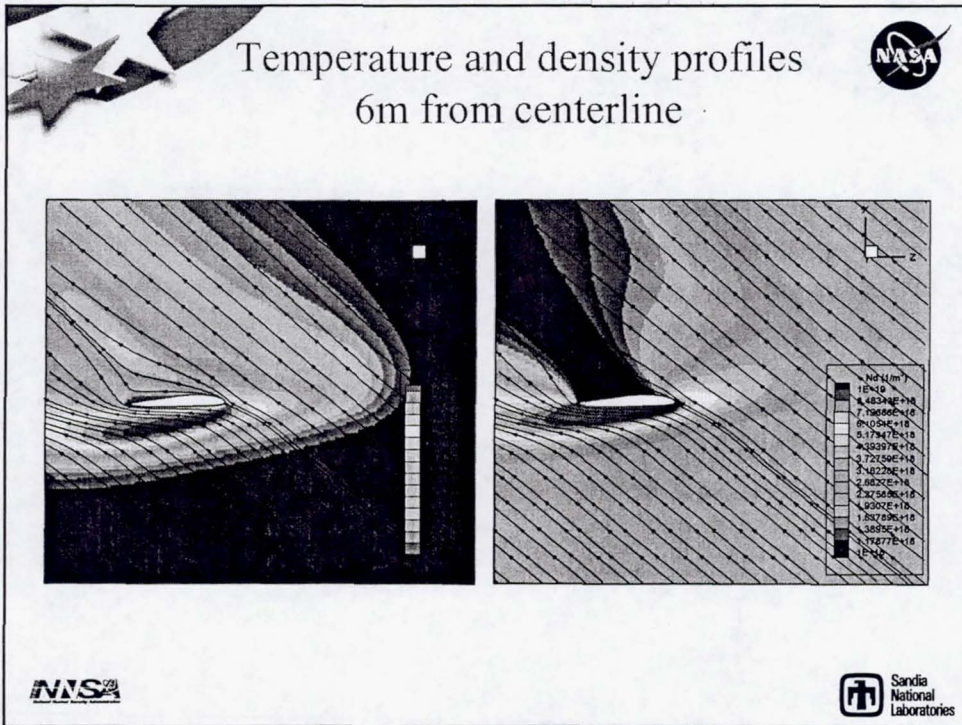
DSMC Point AA	DSMC Point A
EI + 91 seconds	EI + 197 seconds
Mach = 25.1	Mach = 27.0
Altitude = 350,274 ft	Altitude = 300,003 ft
AOA = 41 degrees	AOA = 40 degrees
Kn ~ 0.02	Kn ~ 0.001

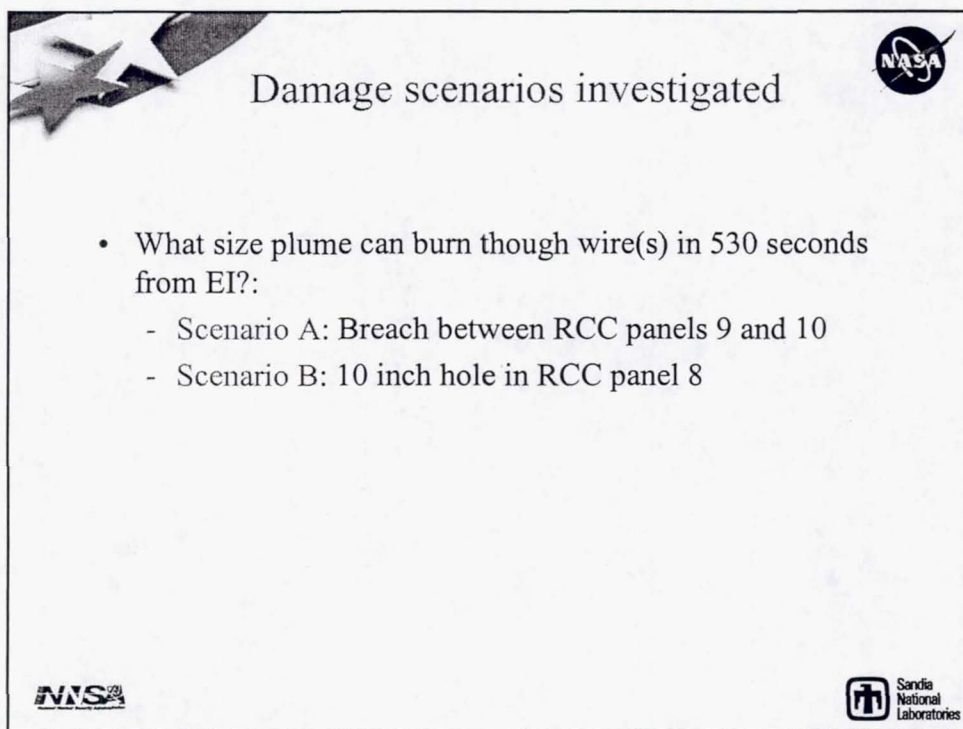
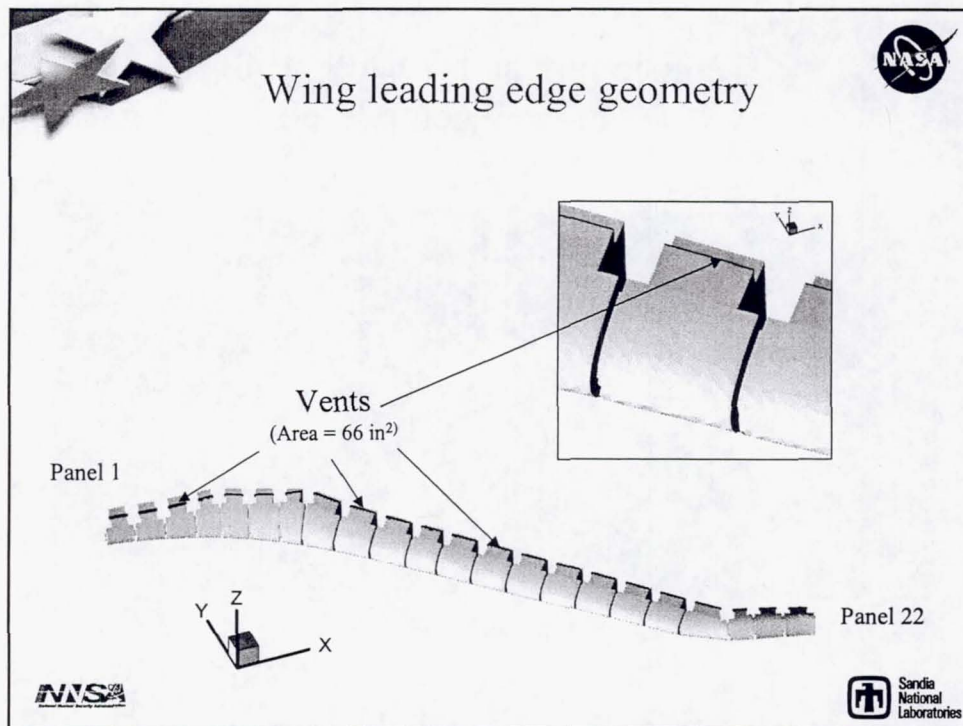


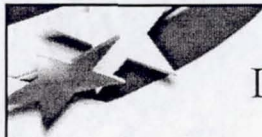










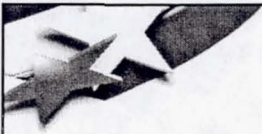


Damage scenarios simulations

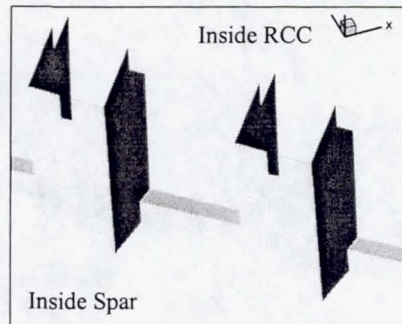
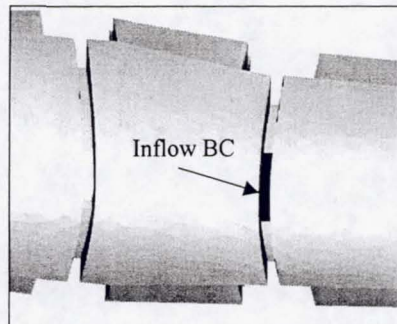


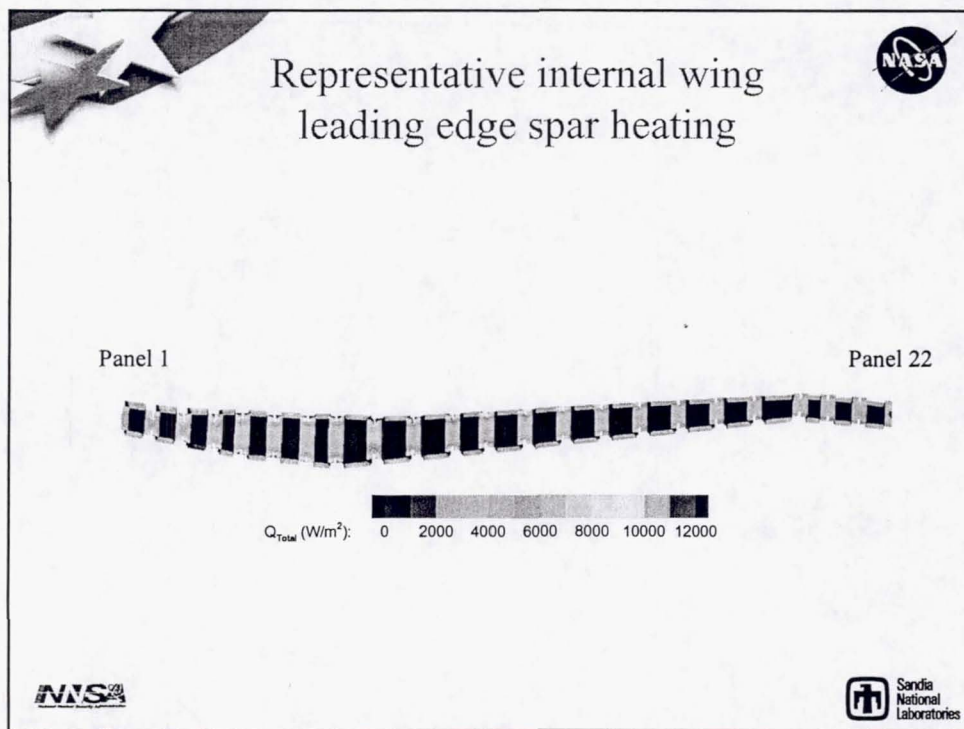
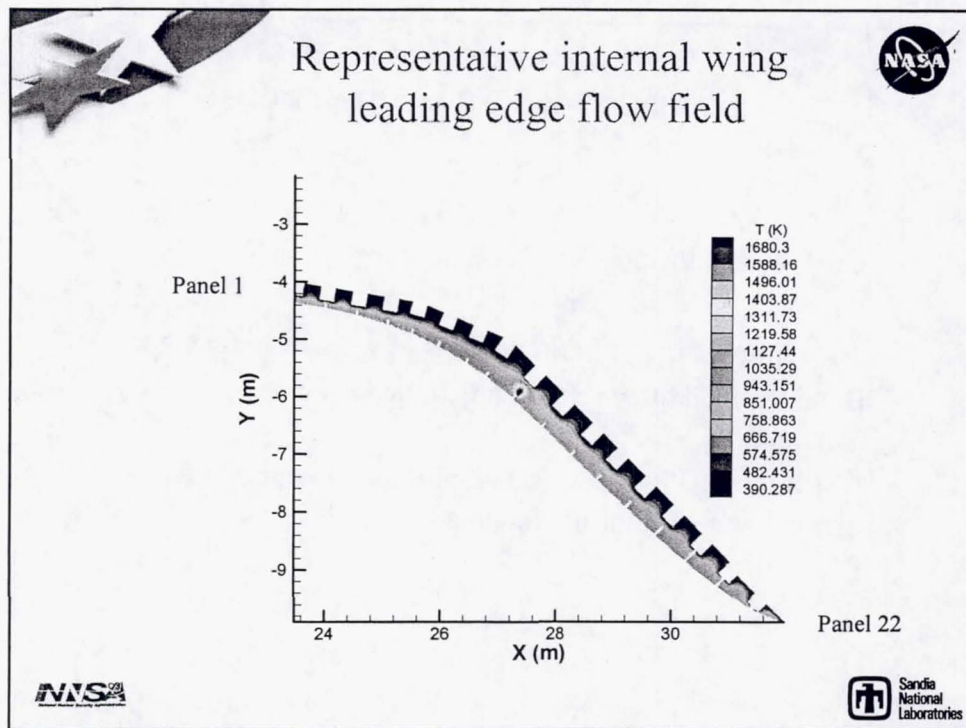
Goal: Model the effects of a damage to the leading edge

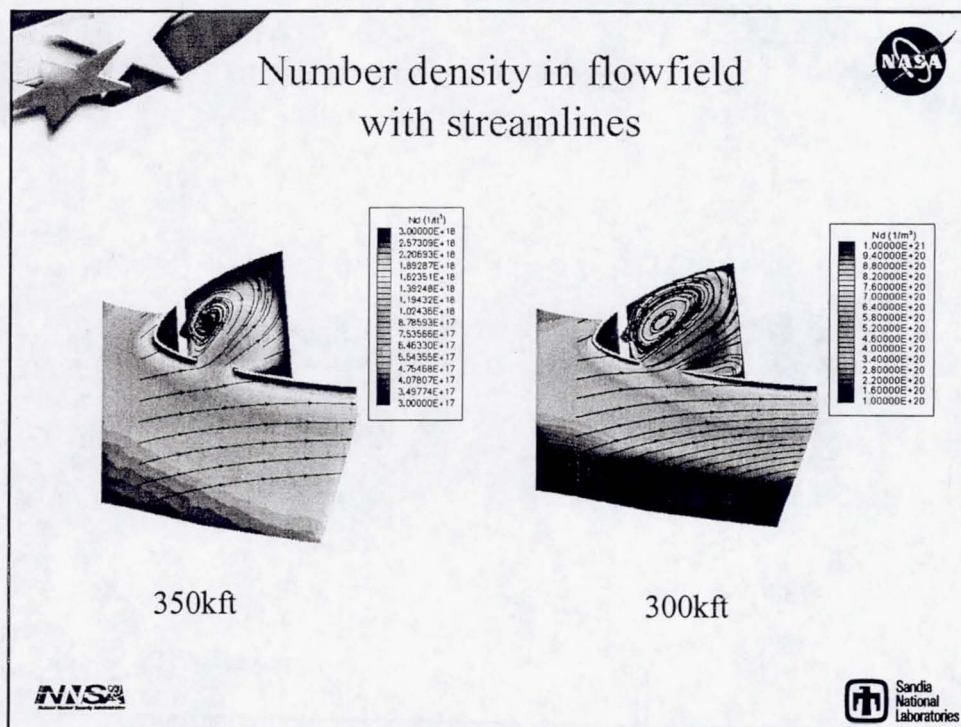
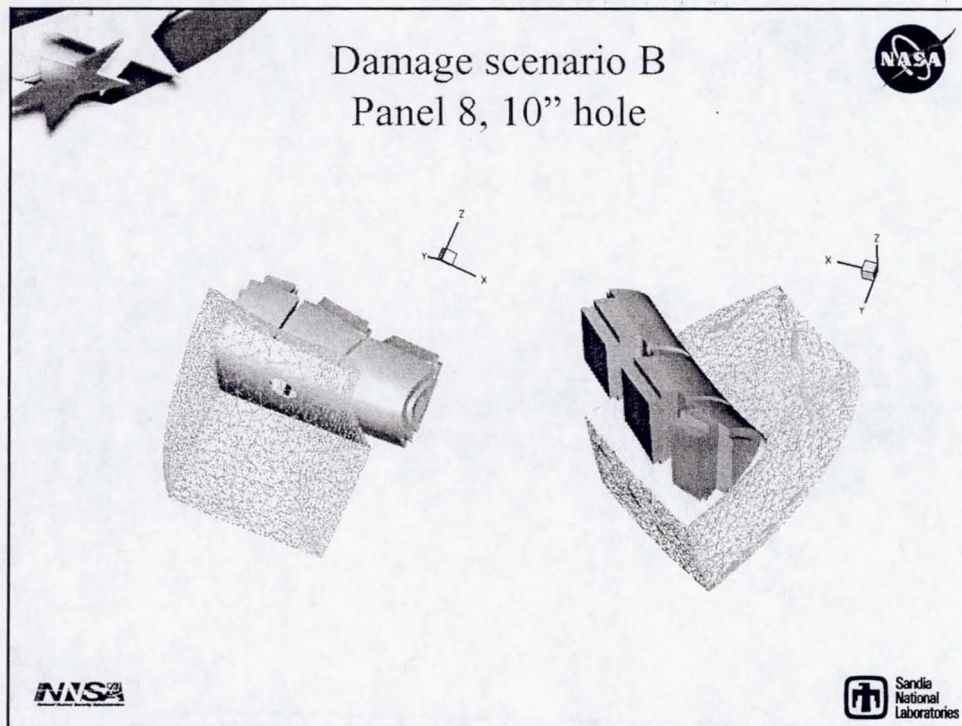
- 3-D representation of critical parts of wing leading edge
- Boundary conditions from undisturbed geometry simulations
- DSMC simulations performed with full chemical and thermal non-equilibrium included

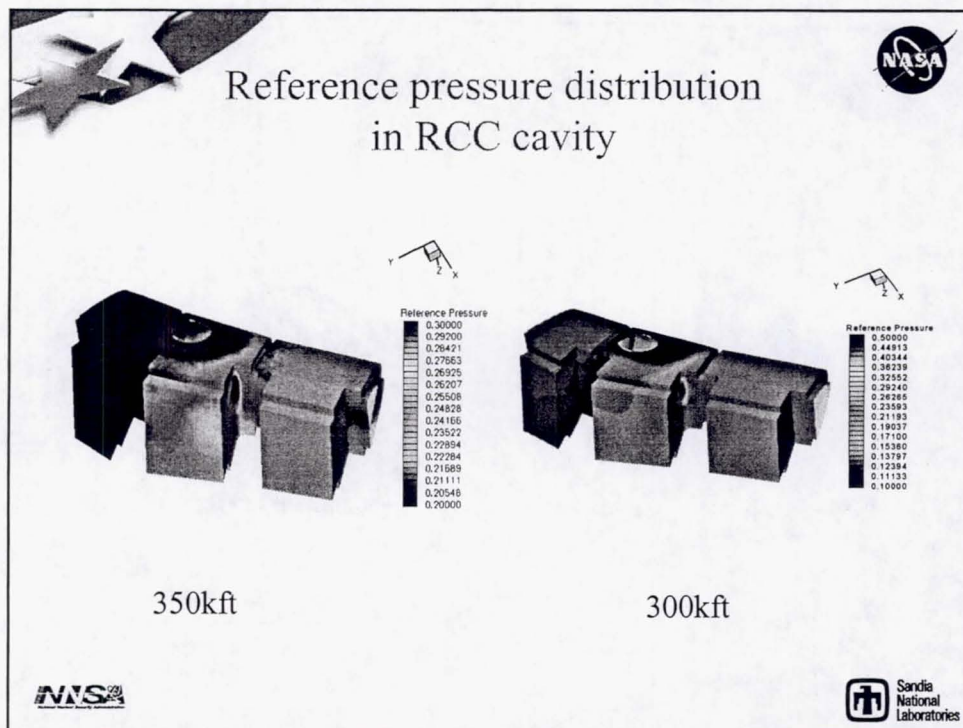
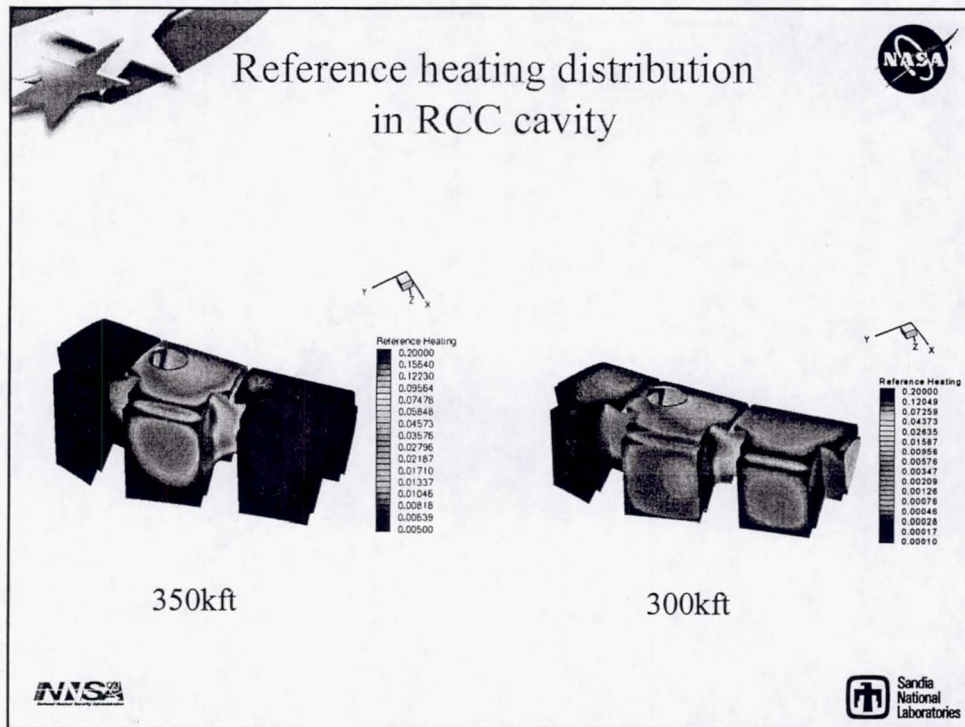


Damage scenario A Flow through a slit







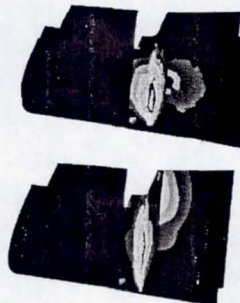


Heating Distribution and Engineering Model Comparisons

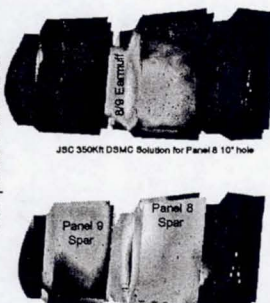


- Plume heating model was developed based on continuum flow assumptions, leading to slightly less diffuse plume structures
- Results are favorable
 - Heating predictions within factor of 2
 - Similar predicted impingement location

Normalized Distributions



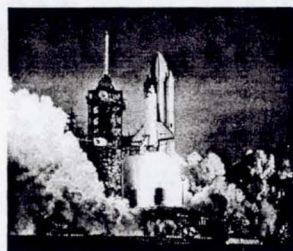
Computed Heat Rate

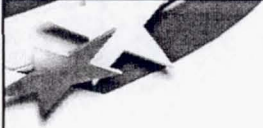


Conclusions







- The Direct Simulation Monte Carlo method was used to provide 3-D simulations of the early entry phase of the Shuttle Orbiter
- Undamaged and damaged scenarios were modeled to provide calibration points for engineering “*bridging function*” type of analysis
- Currently the simulation technology (*software and hardware*) are mature enough to allow realistic simulations of three dimensional vehicles








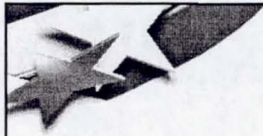
Extras



Applications of DSMC and typical length-scales

- Hypersonics (m)
- Microelectronics manufacturing processes (cm)
- Physical, Chemical vapor deposition (cm)
- MEMS (microns)
- Non-equilibrium chemistry (atomic level)





The limitations of DSMC

- The computational load increases with the density of the flow
- Statistical error decreases as a function of the *square root* of the number of samples
- DSMC can carry more information than actually needed for some applications
- DSMC is an MMP empowered technology



Calculations performed

- 350 kft
 - 2 levels of adaptation
 - 1st level of adaptation: mean free path wide subcells
 - 2nd level of adaptation: 0.5 mean free path subcells
- 300 kft
 - 2 levels of adaptation
 - 2nd level of 350kft adaptation
 - 3rd level of adaptation:(0.1 mean free path subcells)





Grid 6 meters from the centerline

